Urea, (3-methylphenyl)-
63-99-0 DTXSID1075351

Model Performance

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Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75	5%)	Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.08

Global applicability domain: Inside

Local applicability domain index: 5.71e-01

Confidence level: 7.61e-01

Nearest Neighbors from the Training Set

Image not found

Urea, (3-methylphenyl)-

Measured: 1.29 Predicted: 1.08

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1-Phenylurea
Measured: 0.83

Predicted: 1.20

Image not found

Phenacemide

Measured: 0.87 Predicted: 7.52e-01

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Urea, 1-(p-fluorophenyl)-

Measured: 1.04 Predicted: 1.08 Image not found

Urea, (m-fluorophenyl)-

Measured: 1.29 Predicted: 1.07